

4-Aminoacridine
578-07-4 | DTXSID80206487

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.96e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.11e-01

Confidence level: 3.67e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Nabam-sodium</div> <div>Measured: 7.80e-01</div> <div>Predicted: 2.66e-01</div>	<div>Image not found</div> <div>1,5-Naphthalenediamine</div> <div>Measured: 2.40e-03</div> <div>Predicted: 6.55e-03</div>	<div>Image not found</div> <div>4-Aminoacridine</div> <div>Measured: 6.00e-05</div> <div>Predicted: 1.96e-02</div>
<div>Image not found</div> <div>1,8-Naphthalenediamine</div> <div>Measured: 5.37e-03</div> <div>Predicted: 5.83e-03</div>	<div>Image not found</div> <div>Proflavin</div> <div>Measured: 2.39</div> <div>Predicted: 4.01e-02</div>	